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Title: Simulation of etch pit formation through active sites in carbon fiber micro-structures.

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Erosion of carbon due to oxidation does not occur uniformly but through localized etch pit formation as a result of active surface sites [1]. In this work we demonstrate a newly developed capability to capture pitting of carbon fiber microstructures such as FiberForm, which is commonly used as the base material for NASA's spacecraft ablative thermal protection systems (TPS). The simulations are performed at the meso-scale in order to capture the pit formation and growth using direct simulation Monte Carlo (DSMC), specifically using the Stochastic PArallel Rarefied-gas Time-accurate Analyzer (SPARTA) code [2]. Legacy and latest models both assume uniform reactivity of carbon surface sites with oxygen even at the meso-scale level. However, in reality the carbon surface has locally different reaction rates due to the presence of defects at the atomic scale [1]. The defective nature of these sites enhances their reactivity with atmospheric gases compared to the non-defective sites (2-3 orders of magnitude) and are termed as "active sites". Thus, these sites tend to be the first to react and eventually get removed through the formation of gasses such as CO, CO_2, and CN. Their removal results in all the neighboring atoms becoming defective, thus leading to chain reaction of localized carbon removal and formation of etch pits. Capturing the formation of pits during the ablation simulation of carbon micro-structures is critical to predicting their structural failure. Recently a detailed surface chemistry framework was developed in SPARTA, capable of incorporating various reaction mechanisms such as adsorption, desorption, Eley-Rideal (ER) and Langmuir-Hinshelwood (LH) mechanisms [3]. We have implemented the capability of a single surface having multiple site sets with different reactivities within this framework. We have used this feature to model the presence of active sites on carbon surfaces, whose reactivity is orders of magnitude higher than that of the passive sites due to the presence of defects. The active site fraction is a property of surface elements within SPARTA and is directly proportional to the local reactivity of each surface element. By introducing an initial distribution of the active site fraction across the carbon surface and propagating it in a manner that mimics the evolution of real reacting carbon surfaces, we can capture the formation and growth of etch pits as a result of surface consumption reactions such as oxidation.

[1] Francesco Panerai et al. "Flow-Tube Oxidation Experiments on the Carbon Preform of a Phenolic-Impregnated Carbon Ablator". In: Journal of Thermophysics and Heat Transfer 28.2 (2014).
[2] SJ Plimpton et al. "Direct simulation Monte Carlo on petaflop supercomputers and beyond". In: Physics of Fluids 31.8 (2019), p. 086101.
[3] Krishnan Swaminathan Gopalan and Kelly A Stephani. "Development of a detailed surface chemistry framework in DSMC". In: 2018 AIAA Aerospace Sciences Meeting. 2018.